Terephthalic acid, isobutyl 4-nitro-3-methylbenzyl ester

Inchi: InChI=1S/C20H21NO6/c1-13(2)11-26-19(22)16-5-7-17(8-6-16)20(23)27-12-15-4-9-18(21

InchiKey: BUPQUVKASKKNIF-UHFFFAOYSA-N

Formula: C20H21NO6

SMILES: Cc1cc(COC(=O)c2ccc(C(=O)OCC(C)C)cc2)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 371.38

Physical Properties

Property code	Value	Unit	Source
gf	-121.28	kJ/mol	Joback Method
hf	-523.12	kJ/mol	Joback Method
hfus	47.88	kJ/mol	Joback Method
hvap	101.17	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.073		Crippen Method
mcvol	277.440	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	1029.28	K	Joback Method
tc	1276.97	K	Joback Method
tf	678.49	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.56	J/mol×K	1029.28	Joback Method
cpg	884.21	J/mol×K	1070.56	Joback Method
cpg	892.35	J/mol×K	1111.84	Joback Method
cpg	899.01	J/mol×K	1153.13	Joback Method
cpg	904.24	J/mol×K	1194.41	Joback Method
cpg	908.08	J/mol×K	1235.69	Joback Method
cpg	910.57	J/mol×K	1276.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416100&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume